Lecture 06 Quantum Tunneling (1D-case)
Quantum Tunneling (1D Case)

\[ V(x) = \begin{cases} V_0 & , \\ 0 & , \end{cases} \quad 0 < x < a \]
\[ \begin{cases} 0 & , \\ x < 0, x > a \end{cases} \]

In classical physics, \( E < V_0 \) bounced
\( E > V_0 \) penetrating

In quantum physics, penetrating probability depends on \( E, V_0 \) and \( a \).

\[ E < V_0 \quad \text{When} \quad x < 0, \text{or} \ x > a, \]

\[ V(x) = 0 \Rightarrow (-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + 0)\Psi = E\Psi \quad \text{(Schrodinger Equation)} \]
\[ \frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0, \]
\[ \frac{d^2\psi}{dx^2} + k^2\psi = 0 \]

\[ \begin{cases} \text{In} \ x < 0 \ \text{region}, \ \Psi_1(x) \rightarrow e^{ikx} + Re^{-ikx} \quad \text{(reflection)} \\
\text{In} \ x > a \ \text{region}, \ \Psi_\text{III}(x) \rightarrow Se^{ikx} \quad \text{(transmission)} \end{cases} \]
Quantum Tunneling (1D Case)

When \( 0 < x < \alpha \), (Classical forbidden region)

\[
V = V_0 \Rightarrow \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_0\right)\psi = E\psi \quad \text{(Schrodinger Equation)}
\]

\[
\frac{d^2}{dx^2} \psi - \alpha^2 \psi = 0
\]

\[
\psi_{II}(x) = Ae^{\alpha x} + Be^{-\alpha x}
\]

at \( x = 0 \), \( \psi_I(0) = \psi_{II}(0) \) and \( \frac{d\psi_I(x)}{dx}|_{x=0} = \frac{d\psi_{II}(x)}{dx}|_{x=0} \)

\[
\begin{cases}
1 + R = A + B \\
nk(1 - R) = \alpha(A - B)
\end{cases}
\]

\[
A = \frac{1}{2} \left[ \left(1 + \frac{ik}{\alpha}\right) + R \left(1 - \frac{ik}{\alpha}\right) \right]
\]

\[
B = \frac{1}{2} \left[ \left(1 - \frac{ik}{\alpha}\right) + R \left(1 + \frac{ik}{\alpha}\right) \right]
\]

\(
(1)
\)
Quantum Tunneling (1D Case)

since \( \psi_{ll}(a) = \psi_{lll}(a) \) and \( \frac{d\psi_{ll}(x)}{dx} |_{x=a} = \frac{d\psi_{lll}(x)}{dx} |_{x=a} \)

\[
\begin{align*}
Se^{ika} &= Ae^{\alpha a} + Be^{-\alpha a} \\
Ske^{ika} &= Aae^{\alpha a} - Bae^{-\alpha a}
\end{align*}
\]

\[
\begin{align*}
A &= \frac{S}{2} \left(1 + \frac{ik}{\alpha}\right) e^{ika - \alpha a} \\
B &= \frac{S}{2} \left(1 - \frac{ik}{\alpha}\right) e^{ika + \alpha a}
\end{align*}
\]

Combining (1) and (2), we obtain

\[
\begin{align*}
\left(1 + \frac{ik}{\alpha}\right) + R \left(1 - \frac{ik}{\alpha}\right) &= S \left(1 + \frac{ik}{\alpha}\right) e^{ika - \alpha a} \\
\left(1 - \frac{ik}{\alpha}\right) + R \left(1 + \frac{ik}{\alpha}\right) &= S \left(1 - \frac{ik}{\alpha}\right) e^{ika + \alpha a}
\end{align*}
\]
Quantum Tunneling (1D Case)

\[
\frac{S e^{ika-\alpha a} - 1}{S e^{ika+\alpha a} - 1} = \frac{(1 - \frac{ik}{\alpha})^2}{(1 + \frac{ik}{\alpha})^2}
\]

\[
S e^{ika} = \frac{-2i \frac{k}{\alpha}}{(1 - (\frac{k}{\alpha})^2) \sin h(\alpha a) - 2i \frac{k}{\alpha} \cos h(\alpha a)}
\]

\[
T = |S|^2 = \frac{4k^2 \alpha^2}{(k^2 - \alpha^2)^2 \sin h^2(\alpha a) + 4k^2 \alpha^2 \cos h^2(\alpha a)}
\]

\[
= \frac{4k^2 \alpha^2}{(k^2 + \alpha^2)^2 \sin h^2(\alpha a) + 4k^2 \alpha^2}
\]

\[
= (1 + \frac{(k^2 + \alpha^2)^2}{4k^2 \alpha^2} \sin h^2\alpha a)^{-1}
\]

\[
= (1 + \frac{1}{E \frac{V_0}{(1 - E \frac{V_0})}} \sin h^2\alpha a)^{-1}
\]

\[
|R|^2 = 1 - |S|^2 = \frac{(k^2 + \alpha^2)^2 \sin h^2\alpha a}{(k^2 + \alpha^2)^2 \sin h^2\alpha a + 4k^2 \alpha^2}
\]
Quantum Tunneling (1D Case)

If \((aa) \gg 1\), \(\sin haa \sim \frac{1}{2} e^{\alpha a} \gg 1\)

\[
T = \frac{16k^2\alpha^2}{(k^2 + \alpha^2)^2} e^{-2\alpha a}
\]

\[
= \frac{16E(V_0 - E)}{V_0^2} \exp\left(-\frac{2a}{\hbar} \sqrt{2m(V_0 - E)}\right)
\]
Quantum reflection, transmission and tunneling effects

We considered the simplest potential in the form of a rectangular barrier, as shown in the Figure below:

\[ V(z) = \begin{cases} 
V_b, & \text{for } |z| \leq L/2, \\
0, & \text{for } |z| > L/2, 
\end{cases} \]

where \( V_b \), the barrier height, is greater than zero, and \( L \) is the barrier width.
There exist two distinct energy intervals, where the behavior of particle is expected to exhibit different characteristics depending on which energy interval the particle’s energy is in: $0 < \varepsilon < V_b$ and $\varepsilon > V_b$. In classical physics, for the first energy interval, obviously the reflection coefficient is $R = 1$, while the transmission coefficient is $T = 0$; for the second energy interval $R = 0$ and $T = 1$.

In wave mechanics we have to solve the equation

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dz^2} + V(z) - \varepsilon\right] \psi(z) = 0$$

with the potential

$$V(z) = \begin{cases} 
V_b, & \text{for } |z| \leq L/2 \\
0, & \text{for } |z| > L/2 \end{cases}.$$
The solutions are
\[ \psi(z) = \begin{cases} 
    e^{ikz} + re^{-ikz}, & z \leq -L/2 \\
    ae^{-\kappa z} + be^{\kappa z}, & -L/2 \leq z \leq L/2 \\
    te^{ikz}, & z \geq L/2
\end{cases} \]

At the left of the barrier we introduce the incident wave with a unit magnitude, $e^{ikz}$, and a reflected wave, $re^{-ikz}$. At the right of the barrier there is only a transmitted wave, $te^{ikz}$. Then, the exponential factors are

\[ k = \sqrt{\frac{2m_0\varepsilon}{\hbar}} \quad \text{and} \quad \kappa = \sqrt{\frac{2m_0(V_b - \varepsilon)}{\hbar}}. \]

For $\varepsilon < V_b$, $\kappa$ is a real number, and for $\varepsilon > V_b$, $\kappa$ is imaginary number. The parameters $r$, $a$, $b$, and $t$ are still arbitrary functions of $\varepsilon$, which we find by matching these solutions and their derivatives at the walls of the well, $z = \pm L/2$.

The fluxes at $z \to \pm \infty$ can be calculated in terms of $r$ and $t$: $i_{in} = 1, i_r = |r|^2$, and $i_t = |t|^2$. 
Omitting the procedure of calculation of $r$ and $t$, we write down the obvious relationship:

$$R + T = 1,$$

and two different results for the two energy intervals are as follows:

$$T = \frac{1}{1 + \left(\frac{k^2 + \kappa^2}{2k\kappa}\right)^2 \sinh^2 2\kappa L}, \quad \varepsilon < V_b,$$

$$T = \frac{1}{1 + \left(\frac{k^2 - \kappa^2}{2k\kappa}\right)^2 \sin^2 2KL}, \quad \varepsilon > V_b.$$

In the latter formulas we used $K^2 = -\kappa^2$. 
Let us consider first the case of an energy less than the barrier height, i.e., $\varepsilon < V_b$. Classical results can be obtained formally at the limit of zero Planck’s constant, $\hbar$. Indeed, when $\hbar \to 0$, we obtain

$$\kappa = \frac{\sqrt{2m_0(V_b - \varepsilon)}}{\hbar} \to \infty,$$

$$\sinh 2\kappa L \to \infty$$

and $T \to 0$. That is, no transmission through the barrier occurs, as expected. In reality, this classical result is realized for high and wide barriers ($V_b, L \to \infty$).

However, at finite values of these parameters, we always obtain a finite probability of particle transmission through the barrier, which is, as we discussed previously, the tunneling effect. For $\kappa L \gg 1$, $\sinh 2\kappa L = \frac{1}{2} e^{2\kappa L}$ the second term in the denominator predominates and we can approximate the formula as

$$T \approx \frac{16\kappa^2}{(k^2 + \kappa^2)^2} e^{-4\kappa L}.$$ 

Thus, the tunneling effect is determined primarily by the exponential factor. The probability of finding the particle under the barrier is also exponentially small.
For the second case, corresponding to an energy greater than the barrier height, when classical physics gives strictly $T = 1$, from the quantum-mechanical equation

$$T = \frac{1}{1 + \left(\frac{k^2 - K^2}{2kK}\right)^2 \sin^2 2KL}, \quad \epsilon > V_b,$$

we find that $T$ reaches 1 only at $\sin 2KL = 0$, i.e., at certain “resonant” energies, when $2KL = \pi n$ with $n$ being an integer. Otherwise, $T < 1$ with minima at $2KL = (n + \frac{1}{2}) \pi$. All of this means that there exists a reflection of the particle even at large energies.
Oscillations in $T$ with energy for $\varepsilon > V_b$ are explained by “overbarrier reflection” of the particles.

\[ T = \frac{1}{1 + \left( \frac{k^2 + \kappa^2}{2k\kappa} \right)^2 \sinh^2 2\kappa L}, \quad \varepsilon < V_b, \]

\[ T = \frac{1}{1 + \left( \frac{k^2 - \kappa^2}{2k\kappa} \right)^2 \sin^2 2KL}, \quad \varepsilon > V_b. \]

Figure Dependences of transmission coefficient, $T$, on electron incident energy, $\varepsilon$, for different thicknesses of the barrier, $L$: (a) $L = 10$ Å and (b) $L = 20$ Å. Height of the barrier $V_b = 0.3$ eV.
WKB (Wentzel, Kramers, and Brillouin) Method

\[- \frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + U(x) \psi(x) = E \psi(x)\]

\[k(x) = \frac{1}{\hbar} \sqrt{2m[E - U(x)]}\]

for \( E \geq U(x) \)

\[k(x) = \frac{-i}{\hbar} \sqrt{2m[U(x) - E]} = -i \kappa(x)\]

for \( E \leq U(x) \).

\[\psi(x) \approx \exp \left( \pm i \int_x k(x) \, dx \right)\] (zero-order WKB)

\[\psi(x) \approx \frac{1}{\sqrt{k(x)}} \exp \left( \pm i \int_x k(x) \, dx \right)\] (first-order WKB)
WKB Method (cont’d)

\[\psi_{\text{III}}(x) = \psi_{\text{III}}(0) \exp \left[ -\int_0^x \kappa(x') \, dx' \right] = \psi_{\text{III}}(0) \exp \left\{ -\int_0^x \frac{1}{\hbar} \sqrt{2m \left[ U(x) - E \right]} \, dx \right\} \]

Tunneling probability through a barrier.

\[T = \frac{\psi_{\text{II}}^*(L_B) \psi_{\text{II}}(L_B)}{\psi_{\text{II}}(0) \psi_{\text{II}}(0)} .\]
WKB Method (cont’d)

$$T = e^{\int_{x=0}^{L_B} 2\hbar^{-1} \sqrt{2m^* [U(x) - E]} \, dx}$$

Diagram showing the potential $U(x)$ and wavefunction $\psi(x)$ in different regions I, II, and III.